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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

A summary of the work accomplished under the contract is given.

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ATOMIC COLLISION THEORY

Final Report

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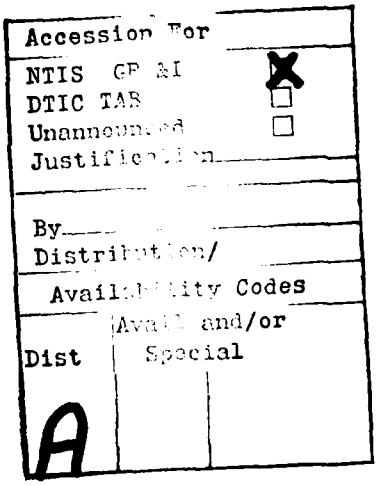

Prepared for the U.S. Office of Naval Research under contract No. N00014-76-C-0041.

The work of the LSU theoretical atomic physics group under this contract was directed originally toward the computation of rovibrational cross sections for electron impact excitation of H_2 and toward the development and improvement of calculational techniques. This theme remained dominant but variations and extensions to diverse topics were developed such as a study of autodetaching states of negative ions or the effect of strong magnetic fields on atoms. In addition, attention was directed towards the calculation of cross sections for electron excitation of oxygen and copper, atoms important in the upper atmosphere of the earth and in laser development, respectively.

The major thrust of the work involved calculations on rotational-vibrational excitation of molecules D_2^+, H_2, and HCl (publications No. 1, 3, 17, 22, 25, 28) and a review of this area (No. 27).

On the subject of development and improvement of calculational techniques, papers were published on a non-iterative integral equation method and its related Green's function (No. 12, 13, 24, 25, 29). Other calculational methods were explored, such as the algebraic variational method (No. 2), a combined R-matrix and variable phase technique (No. 4), the Harris-Nesbet method (No. 5) and a proposed calculational procedure for electron-atom scattering at arbitrary energies (No. 14).

Another major thrust of the work involved calculations on electron impact excitation of atomic oxygen (No. 8, 18, 19, 21, and 24), of atomic fluorine (No. 26), and of atomic copper (No. 30). Finally, an application to excitation of a multicharged ion, NV, was made (No. 20).

In addition to calculations and methods pertaining to the major theme of the contract, a number of studies were made on interesting problems in other subareas of atomic physics. Accurate bound state methods were applied to give a deeper understanding of some experiments on autodetachment states of Li^- and Na^- (No. 6), O^- (No. 11), and $C\ell^-$ (No. 15). The effect of a strong magnetic field was studied for H (No. 9, 10) and for H^- (No. 16). Finally, positronium formation in positron-hydrogen collisions was calculated (No. 7).

There has been considerable progress in the field of electron-molecule scattering in the past ten years. The work supported by this contract has concentrated on the energy region up to 10 eV, and on the processes of rotational and vibrational excitation of diatomic molecules. The standard techniques in which the electron-molecule interaction is expanded in partial waves and electron exchange effects are included explicitly, are very tedious and time consuming. Exchange effects may be included to reasonable accuracy in a local approximation such as that of a free electron gas. Further, it may be possible to solve the problem as a two dimensional one and hence avoid the expansion over a large number of partial waves.

For electron atom scattering, it has become apparent that it is necessary to have an accurate description of the target wave functions before proceeding to the scattering calculations. While our results for e^- Cu disagree with experiment, we are confident that they are internally consistent and correct. A repeat of the very difficult experiment involving copper vapor is eagerly awaited, particularly because of its potential

importance in the development of a green laser which has tolerable efficiencies (~ 1%).

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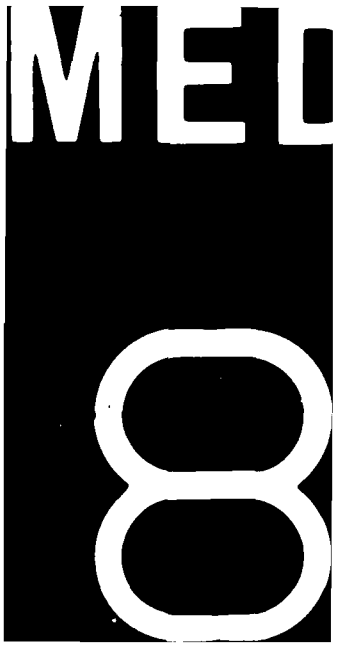
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